Issues in Chemical Processing by Self-Assembly

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UCSB

“Self-assembly is a spontaneous process in which supermolecular hierarchical organization is established in a complex system of interlocking components.”

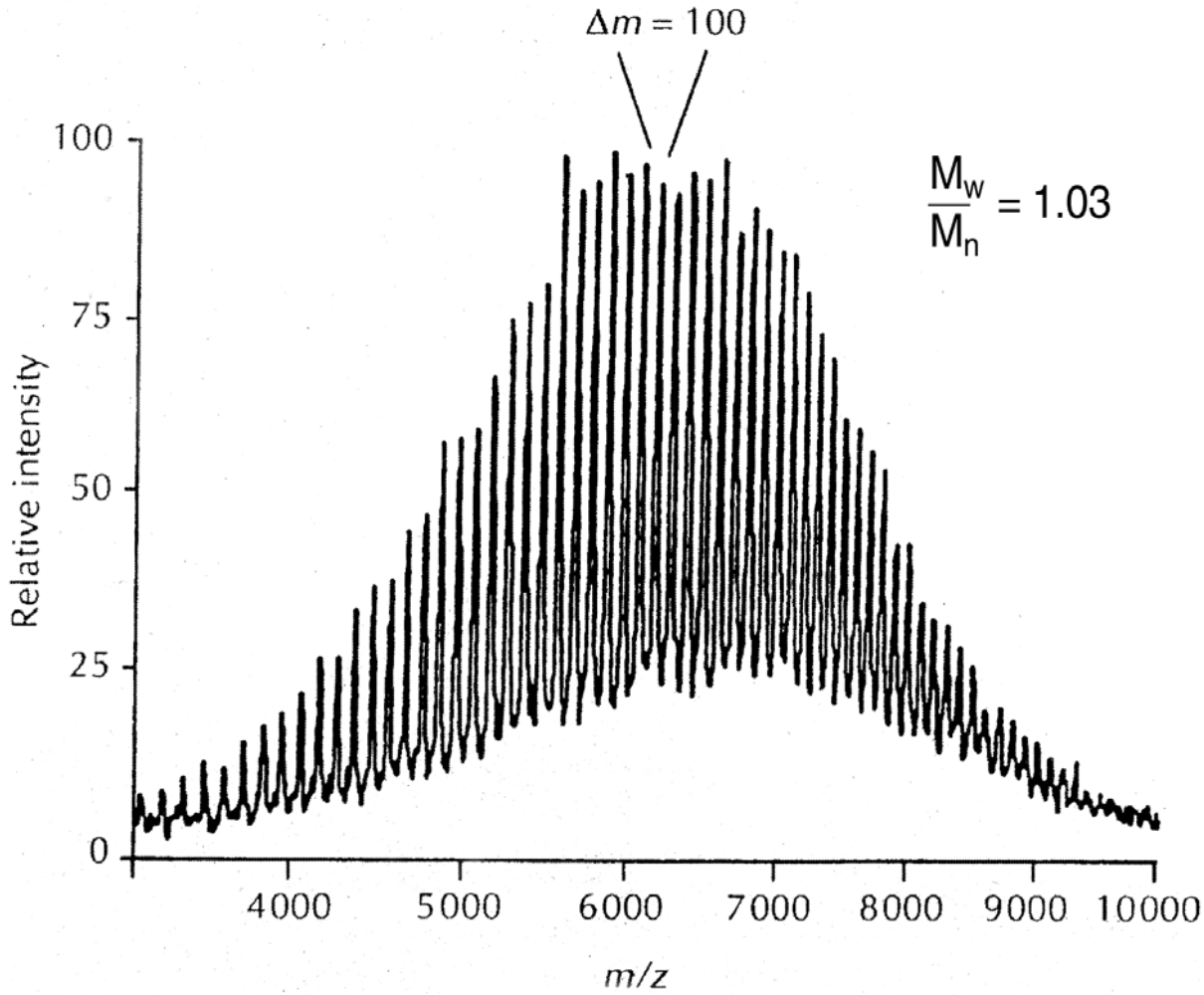
H. Kuhn and A. Ulman

Thin Films

Principles and Issues in Self-Assembly

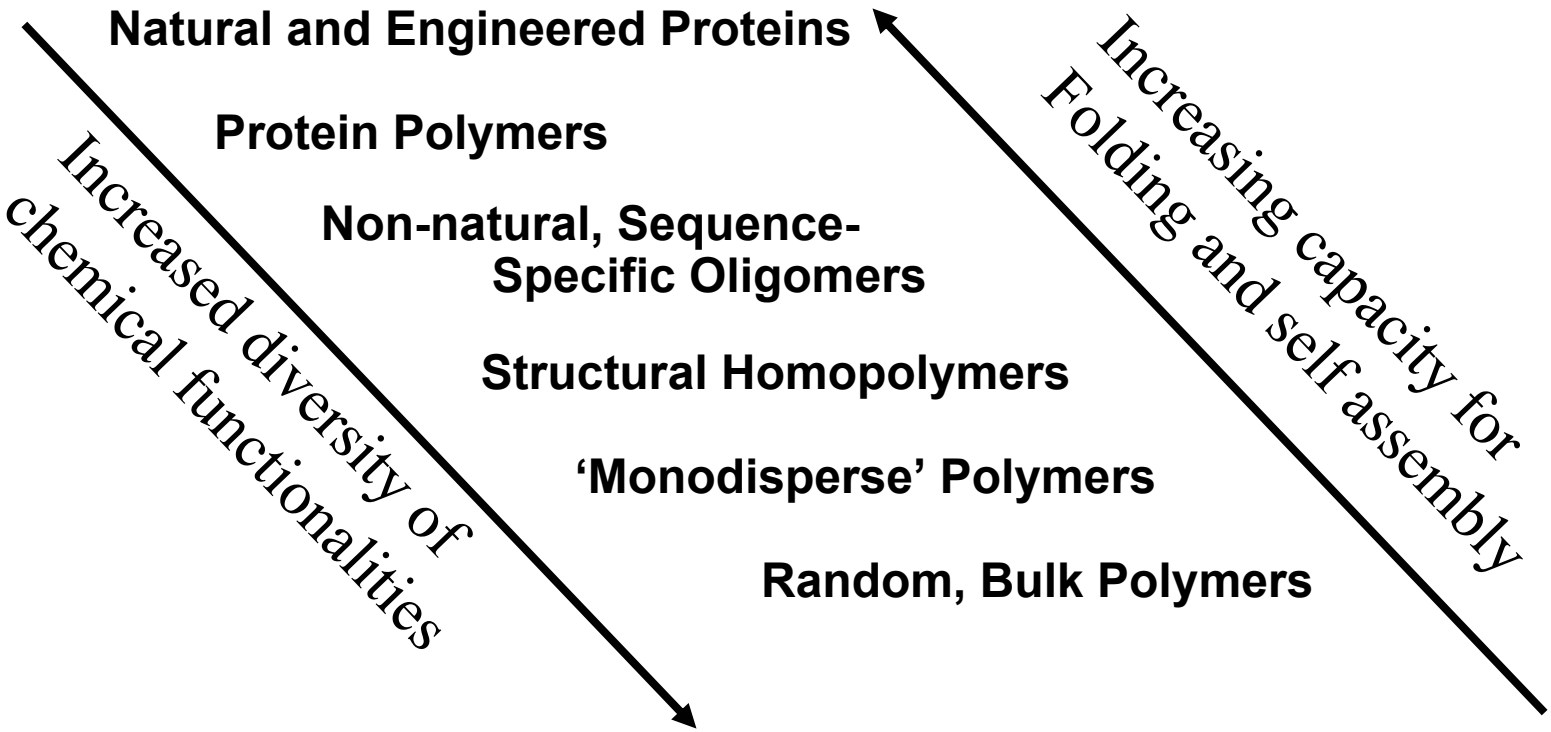
- ***Precision synthesis***
- **Hierarchical structures**
- **Expanding the idea of the molecule**
- **Scalable processing routes with quantifiable and controllable kinetics**

MALDI Mass Spectrum of Poly(methyl methacrylate)



Bahr et al., Anal. Chem. 64, 2866 (1992)

Range of Macromolecular Materials



Must these arrows run in opposite directions?

What capacity is lost as precision and fidelity in synthesis is lost?

Barron & Zuckermann, Curr Opin Chem Biol 3: 681 (1999)

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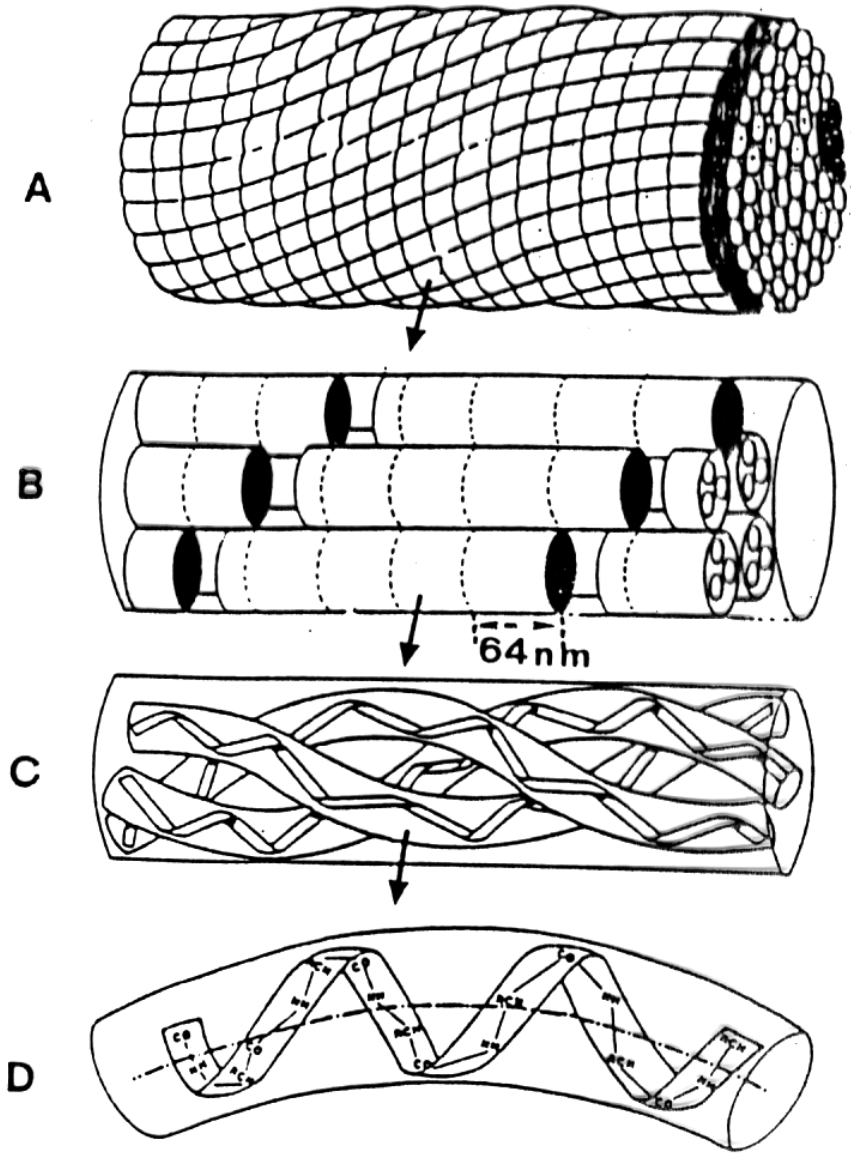
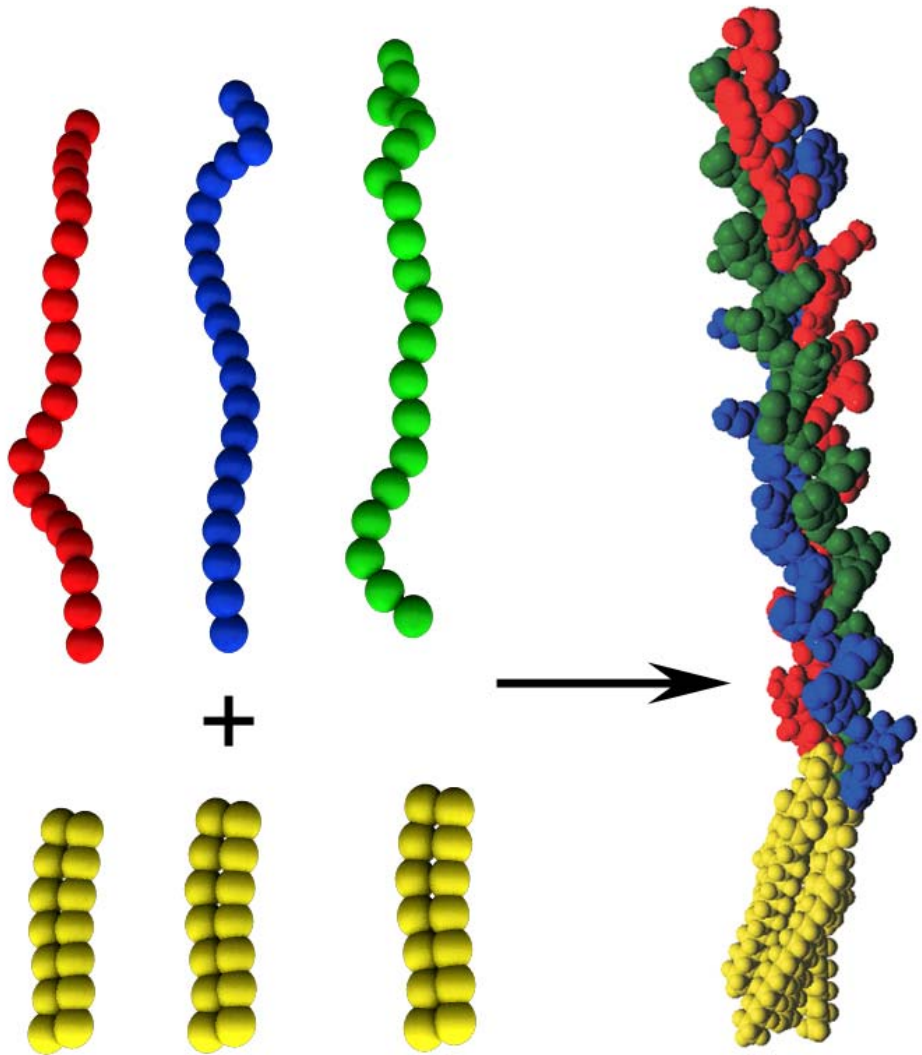
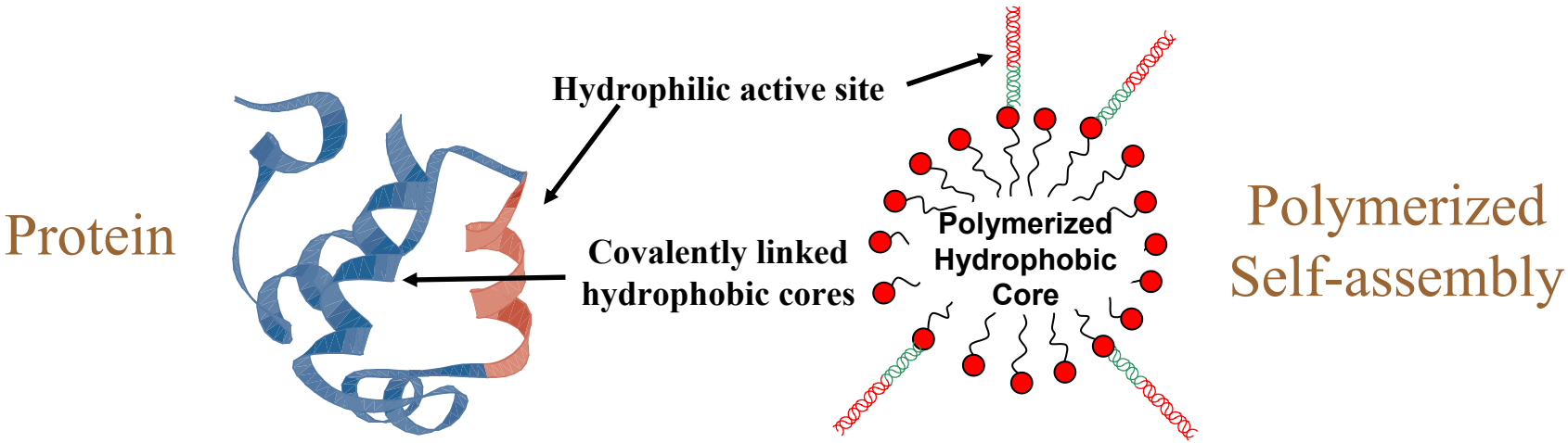


The structure of collagen fibers. A) collagen fiber B) fibril C) tropocollagen D) helical polypeptide. Reproduced from Djabourov et al. (1993)

Peptide Amphiphiles



Protein Analogous Micelles



- **Hydrophobic core and hydrophilic shell**
- **Hydrophilic active site with distinct secondary structure**
- **Active sites orientated outward for bioactivity**
- **Globular (~10 to 100 nm)**
- **Evolve affinity and specificity with combinatorial chemistry**

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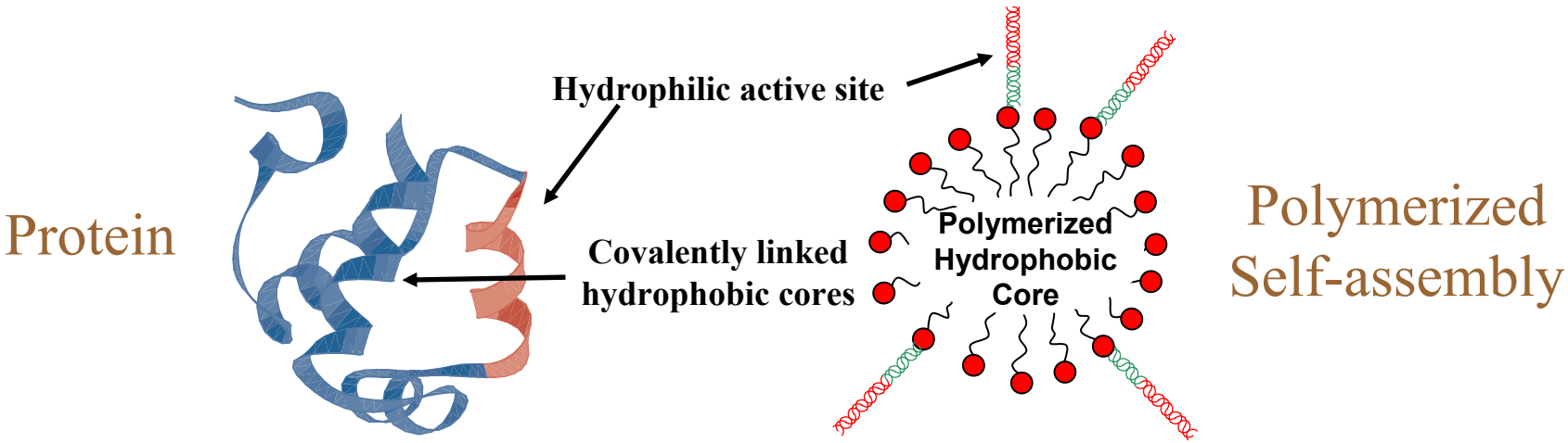

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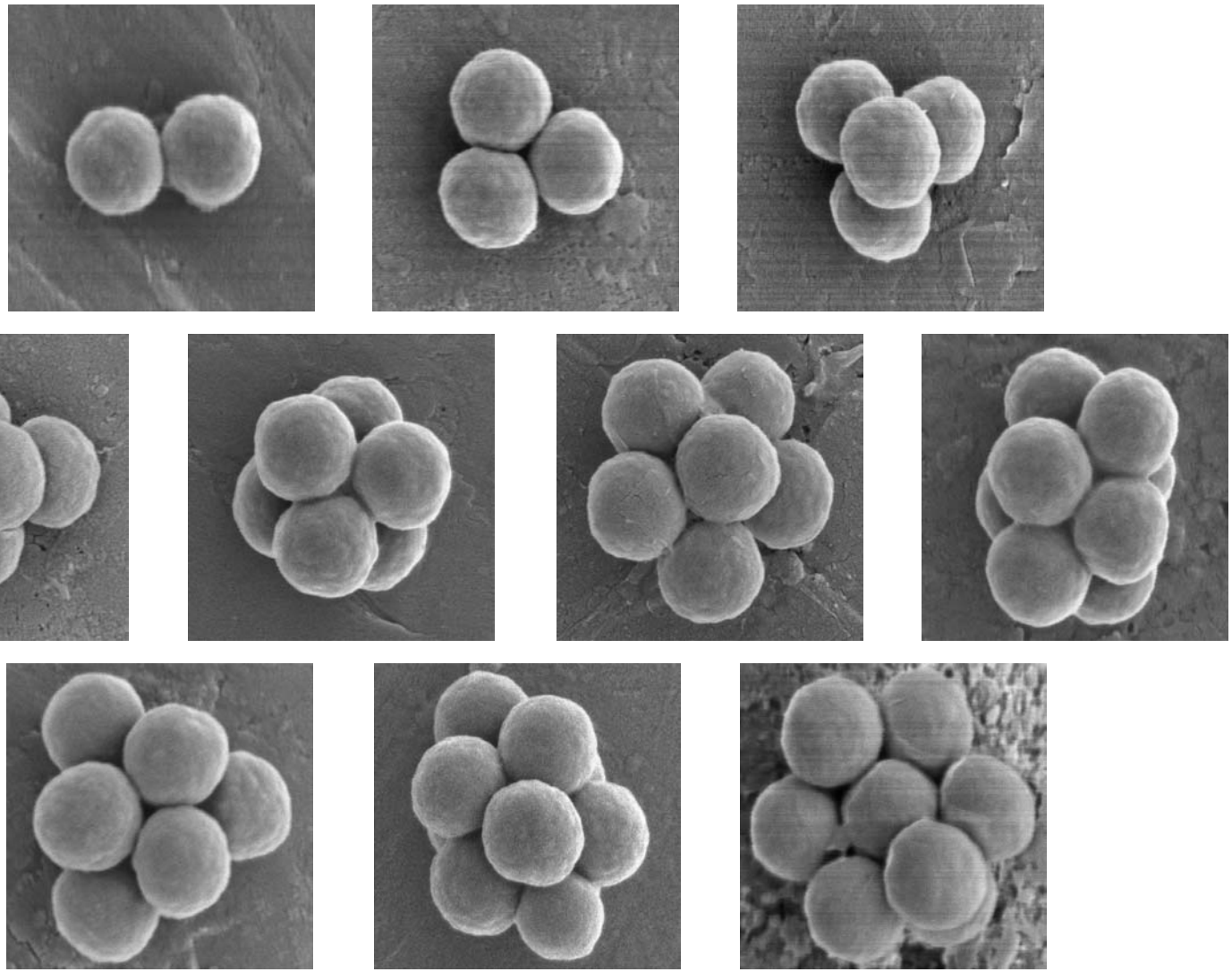
The minimal moment clusters



Predicated by John Conway, Neil Sloane et al

Assembled & measured by Vinny Manoharan

Conferring molecule-like characteristics on supermolecular structures, dendrimers, micelles, objects, particles ...

Self-assembled materials are built on interaction potentials arising from:

- **shape / molecular architecture**
- **packing**
- **electrostatic**
- **solvation**
- **hydrophobic**
- **hydrogen bonding**
- **metal coordination**

controlled arrangement of functional sites

Need to clarify rules of non-covalent bonding; Develop understanding of reaction mechanisms

Principles and Issues in Self-Assembly

- **Precision synthesis**
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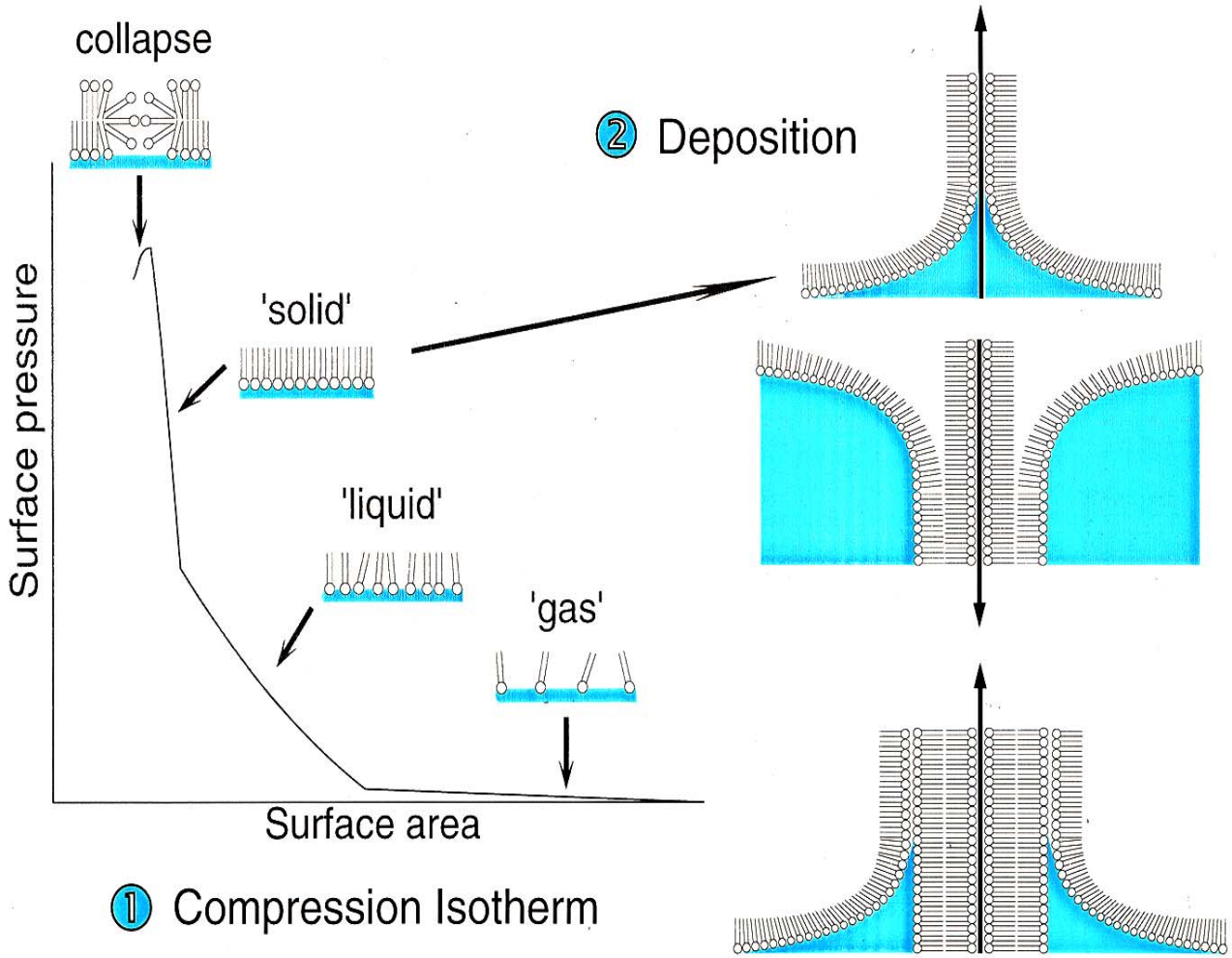
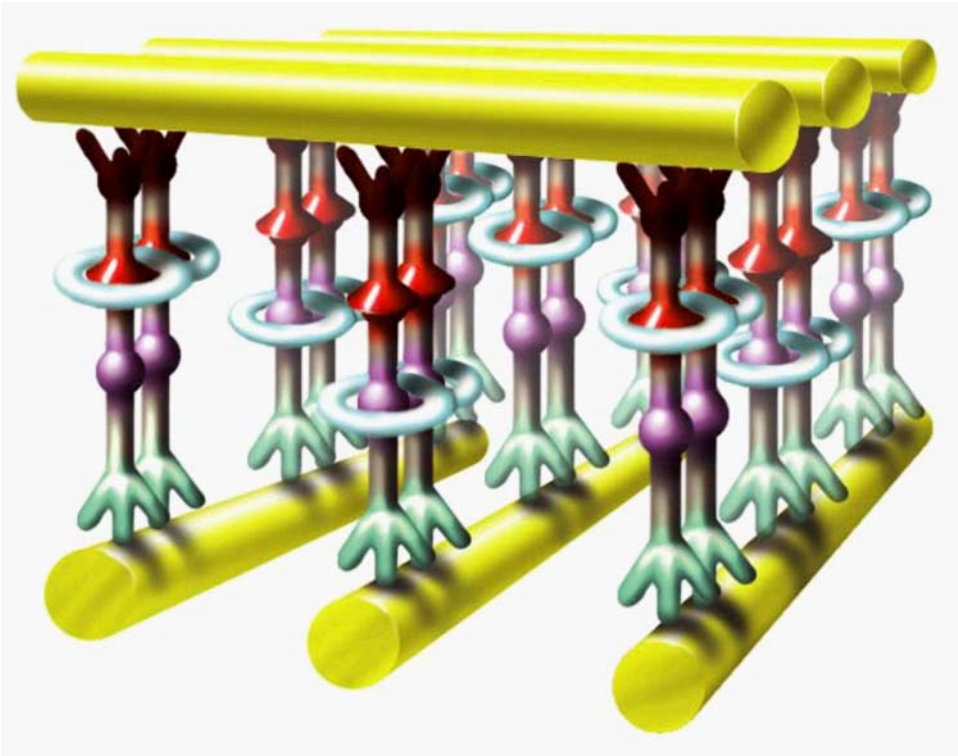
Creating Ordered Surfaces: Langmuir-Blodgett Techniques



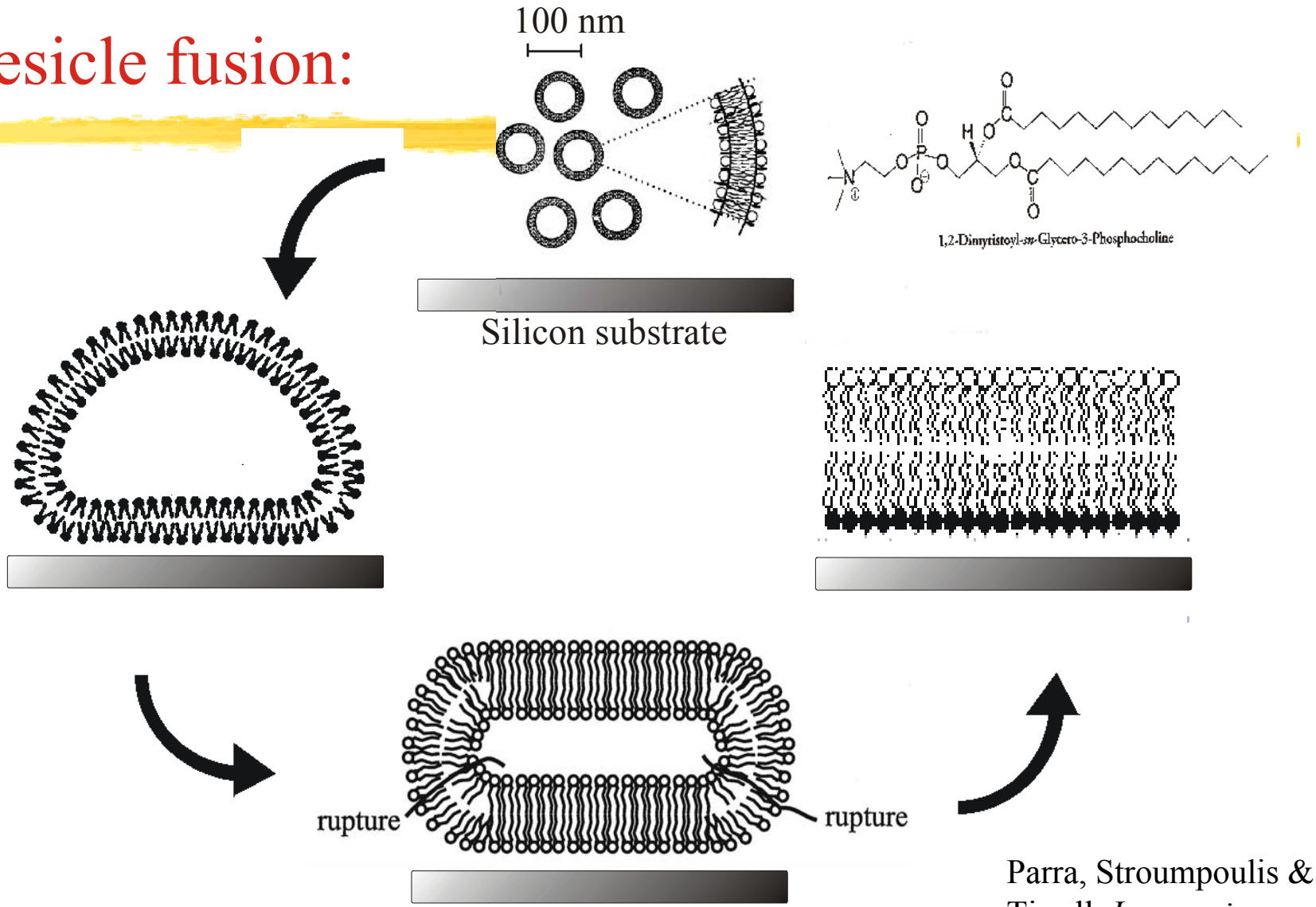
Molecular Memory Circuit



Currents passed between perpendicular nanowires alter the conductivity of organic molecules sandwiched in between.

Heath et al., Science., August 3, 2001, VOL 239

Vesicle fusion:



Parra, Stroumpoulis & Tirrell, *Langmuir,* submitted, 2003

Images taken from:
Leonenko, ZV, et al., Biochim. et Biophys. Acta, 1509 (2000) 131-147.
Reviakine, I. et. al., Langmuir, 16 (2000) 1806-1815.

Important issues/barriers/research opportunities for the future of self-assembly processing

- **Scale-up of precursor production (while respecting need for uniformity in size, shape, composition, distribution of functional chemistry)**
- **Identification of self-assemblers (information content, combinatorial searches)**
- **Kinetics and dynamics of self-assembly (catalysis, templating, influence of fields)**
- **On-line, real-time monitoring and control**
- **Structure-property relationships**
- **Scale-up in size, speed and geometrical complexity**
- ***Self-assembly has strong competition ...***